S. A.
Sect. A

Crystallography

2200.   Finding the coordinates of the atoms in the unit cell of a crystal by means of the Fourier. A. L. Mackay. ... Maper. Tsar. Pis., 21, 717-30 (Ne. 6, 1951) In Russian.

It is shown that the midpoint of any interatomic vector of the Fourier is a centre of inversion which contains two groups of points each of which represents the structure of the crystal. The possibility of uniquely deriving a structure from its representation as a 1-dimensional Fourier has been shown by Burger (Abstr. 3517 (1950), and the practical schedule for doing this which is developed here follows observations by Sundin and Zdanov (Abstr. 9117 (1939). Three-dimensional Fourier are necessary, and a calculation is adduced showing that the practical solution of a structure (all the atoms of which are approximately the same weight) is likely to be possible.

A. L. MACKAY

CA

2

X-ray structure investigation of 1,8-dichloronaphthalene. A. I. Kitaigorodskii and S. S. Kabalkina (Inst. Org. Chem., Moscow). Zhur. Fiz. Khim. 35, 71-81(1961).—The dimensions of the unit cell of 1,8-dichloronaphthalene are: $a = 15.00 \pm 0.1$; $b = 4.10 \pm 0.03$; $c = 14.5 \pm 0.3$ A.; $\beta = 93°55' \pm 5'$; 4 mols. per unit cell; space group C_{2h}^5 ($A2/a$). Two at. coördinates are first detd. from the reflection intensities, then the orientation of the mol. is calcd. and the third coördinates are deduced from it. The structure is verified by the good agreement between the calcd. and exptl. structure amplitudes, F, e.g., for $hkl = 200$, 400, 711, 311, 600, 602, resp., $F_{calcd} = 40, -52, 50, -42, 18, 0$, and $F_{exptl} = 41, 52, 54, 42, 18, 8$. The bond distances are (in A.): C_1-C_2, 1.40; C_2-C_3, 1.23; C_3-C_4, 1.37; C_1-Cl, 1.76; C_4-C_4, 1.20. The error is estd. at ± 0.08 A. These results agree well with the bond distances found for naphthalene (Abrahams, et al., C.A. 44, 13743i). The Cl atom probably displaces C_1 by approx. 0.02 A. which is beyond the exptl. error.   Michel Boudart

1957

CA

Possibility of determining the center of symmetry of a crystal by x-ray structure analysis. A. I. Khaigorodskii. Zhur. Fiz. Khim. 23, 127-8(1961).—This possibility, as shown by Wilson (Acta Cryst. 2, 318(1949)) rests on the fact that $(Fh)/Fh$ is equal to $x/4(0.785)$ when there is no symmetry center and to $2/x$ (0.637) when there is one. There are, however, limiting cases and it is conceivable that the ratio may take any value between 0.637 and 0.785. The method succeeds in proving the absence of the symmetry center but fails in proving its presence. In the work of Llewellin, et al. (C.A. 44, 8730e) crystals known to have a symmetry center give ratios of the order of 0.64-0.70, whereas known noncenter structures give $(Fh)/Fh = 0.76$-0.79. The method fails in nontrivial cases; e.g., the quoted authors assign (C_5H_5)Fe to the space group P_1/c. This is incorrect; as in many analogous cases, the packing of org. mols. in this group is difficult, the 2 axis (thus the inversion center) is lost and the group Pc is formed with 4 mols. (3 noncentr.) per unit cell. The mols. in such a crystal are very densely packed and their arrangement differs only little from a structure possessing an inversion center (cf. C.A. 43, 838c).   Michal Bonders

Chemical Abst.
Vol. 48 No. 8
Apr. 25, 1954
General and Physical Chemistry

C A

2

Crystal structure of iodoform. A. I. Kitaigorodskii, T. L. Khotsyanova, and Yu. T. Struchkov (Inst. Elem. Org. Chem., Acad. Sci. U.S.S.R., Moscow). Doklady Akad. Nauk S.S.S.R. 78, 1161–4 (1951).

Kitaigorodskii, A. I., and Merentsev, V. A.: Atom i
molekula (Atoms and Molecules). Moscow: State Pub.
House Cultural and Ed. Lit. 1952. 76 pp.

(1) *Rev pot*

PHASE I Treasure Island Bibliographic Report

00000032

BOOK
Author: KITAIGORODSKII, A. I.
Full Title: X-RAY STRUCTURAL ANALYSIS OF MICROCRYSTALLINE AND AMORPHOUS SUBSTANCES.
Transliterated Title: Rentgenostrukturnyi analiz melkokristallicheskikh i
                       amorfnykh tel.
Publishing Data:
  Originating Agency: None.
  Publishing House: State Publishing House of Technical-Theoretical Literature.
  Date: 1952.   No. pp.: 588   No. of copies: 6,000
  Editorial Staff   *over*
    Editor: None.   Tech. Editor: None.
    Editor-in-Chief: None.   Appraiser: None.
Text Data
  Coverage: The book which is a continuation of another work by the same author
             entitled X-Ray Structural Analysis, 1950, describes the application of
             X-Ray structural analysis to the study of amorphous and microcrystalline
             substances, irregular crystals, and other substances. Pt.I: X-Ray
             diffraction by amorphous, quasi-crystalline, and polycrystalline substances.
             Pt.II: Data on X-Ray structural analysis (Hydrocarbons and their deriva-
             tives, proteins, cellulose, animal tissues, fats and soap, coal, inorganic
             compounds, metals, and polycrystalline substances). Tables of distances
             between planes and relative intensities of lines in X-Ray graphs for 1299
             polycrystalline substances pp. 417-578). Subject index.
  Purpose: A textbook for engineers and scientific personnel; also, for students of
            advanced courses in technical institutions of higher learning.

CC000032

Card 2/2

Call No.: QD945.K55

Full Title: X-RAY STURCTURAL ANALYSIS OF MICROCRYSTALLINE AND AMORPHOUS SUBSTANCES

Facilities: None.

No. of Russian References: References appear only in footnotes.

Available: Library of Congress.

KLIMENKOV, V.S.; KARGIN, V.A.; KITAYGORODSKIY, A.I.

Density of packing of highly polymeric compounds. Khim. i Fiz.
Khim. Vysokomolekul. Soedineniy, Doklady 7-oy Konf. Vysokomolekul.
Soedineniyam '52, 231-41.   (MLRA 5:7)
(CA 47 no.15:7817 '53)
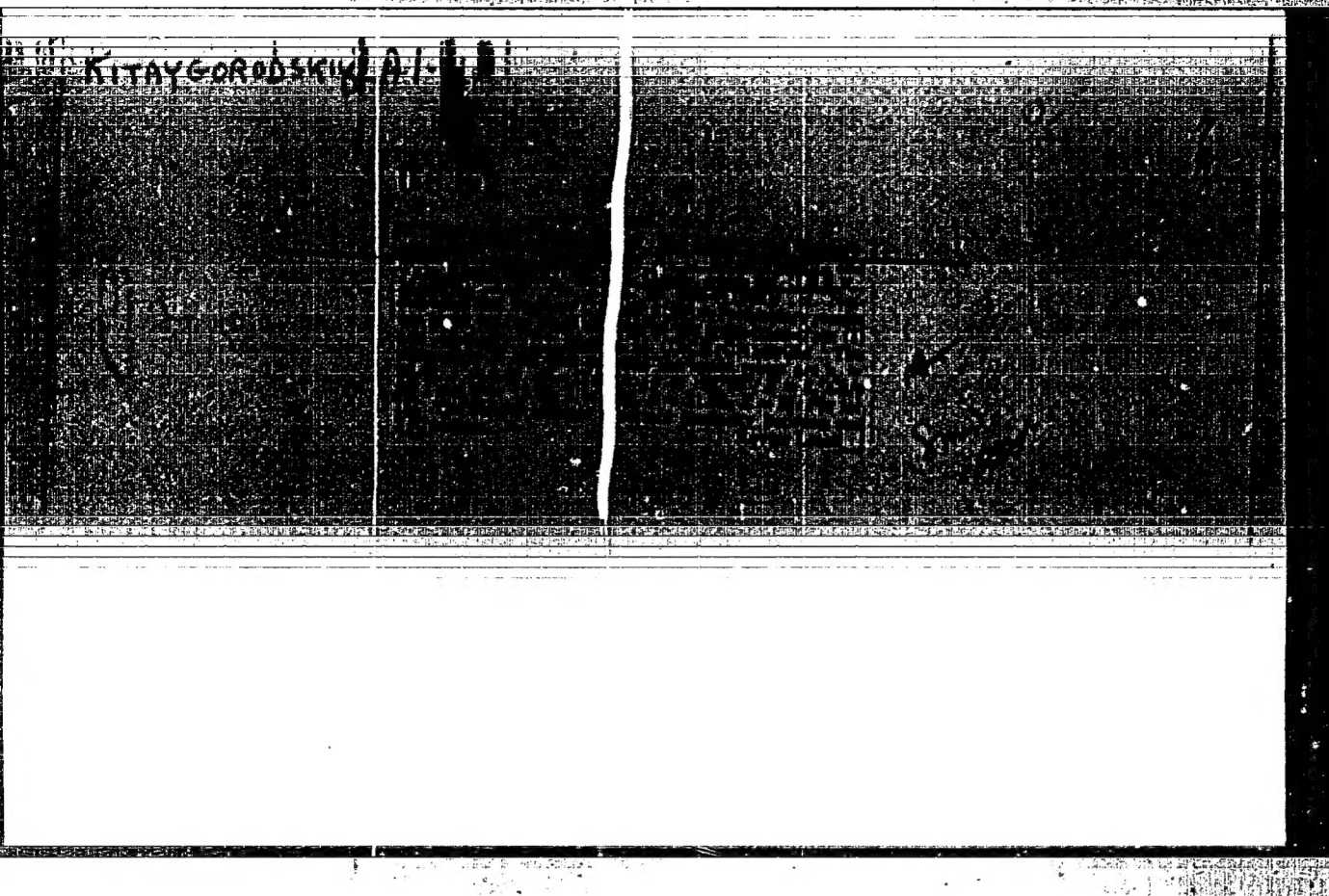
KITAYGORODSKIY

KITAYGORODSKIY, A. I. Prof.

Science

Undertaking of great importance; (On the popular science library of the State Technical Publishing House). Priroda 41, No. 6, 1952.

KITAYGORODSKIY, A.L. PROF.

Symmetry

Something new about symmetry. Pirioda 41 no. 7, 1952

Inst. of Organic Chemistry, AS USSR

KITAYGORODSKIY, A. I.

USSR/Physics - Solid State Physics   Jan 52

"Progress in X-Ray Structural Analysis of Crystals,"
A. I. Kitaygorodskiy

"Uspekh Fiz Nauk" Vol XLVI, No 1, pp 23-70

Brief exposure of theoretical computation of dif-
fraction by cryst lattice with reference to book
by himself (cf. "X-Ray Structural Analysis" 1950).
Defines structure of crystals by interatomic vec-
torn, determines phases of structural amplitudes,
series of electron densities and discusses possi-
bilities of X-ray analysis.

209T103

KITAYGORODSKIY, A. I.

USSR/Physics - Crystals   Jul 52

"New Method of Determination of Complex Structures of Crystals," A. I. Kitaygorodskiy

"Uspekh Fiz Nauk" Vol XLVII, No 3, pp 487-489

Essence of subject method is as follows: from the intensities of the X-ray reflections one calculates the structural amplitudes F_H by the usual familiar procedures and reduces the values of F to an abs scale also by familiar methods; then by usual methods of averaging the mean atomic factors are found, after which one possesses knowledge of the abs magnitudes of unit structural amplitudes U_H for each reflection; that is, amplitudes such that are equal to unity if all atoms scatter in one phase.

225T102

KHOTSYANOVA, T.L.; KITAYGORODSKIY, A.I.; STRUCKHOV, Yu.T.

Crystal structure of tetraiodoethylene, C2I4. Doklady Akad. Nauk
S.S.S.R. 85, 785-8 '52.   (MLRA 5:8)
(CA 47 no.16:7854 '53).

(PA 56 no. 671: 8096 '5)

1. KITAYGORODSKIY, A. I.,   Prof.

2. USSR (600)

4. Molecular Theory

7. Atomic structure of matter. Fiz v shkole No 1   1953.

9. Monthly List of Russian Accessions, Library of Congress, _   April____ 1953, Uncl.

KITAYGORODSKIY, A.I.
Kitaygorodskiy, A.I.

USSR.

543 735

7875. The statistical method of determining the signs of the structure amplitudes. A. I. Kitaigorodskii. Letter in Zh. eksper. teor. Fiz., 24, No. 6, 747-8 (1953) In Russian.

The relationship (sign F_{hkl}) (sign $F_{h'k'l'}$) = (sign $F_{h+h', k+k', l+l'}$) is deduced and an expression for the limits of its validity is derived. If $z = F_{hkl} \cdot F_{h'k'l'} \cdot F_{h+h', k+k', l+l'}$ and $g = 2(\overline{x^3}/\overline{x^2}) - 1)^{-1}$ then W, the probability that z is positive, is given by $1/W = 1 + \exp(-gz/\overline{z})$. The probability that the sign relationship is true is greater when $\overline{x^3}/\overline{x^2}$ is small, the latter term being a minimum when there are heavy atoms in the cell. The signs of strong reflections are almost certain; ie when $|z|$ is large. In the least favourable case of identical atoms the lowest probability for 25 atoms is 85% and for 100 atoms 70%.

A. L. MACKAY

KITAYGORODSKIY, A. I.

7

Low-temperature study of the structure of aromatic compounds. I. Khotsyanova. Thermal expansion of anthracene. V. M. Kozhin and A. I. Kitaygorodskii [text]. Dokl. Akad. Nauk S.S.S.R. ____ Zhur. Fiz. Khim 27, ___ (1953) — X-ray measurements were made on a single crystal. The dimensions of the unit cell at 20° are a = 6.21Å ± 0.005, b = 5.93 ± 0.005, c = 8.45 ± 0.005, β = 122°55' ± 10', at −195° these are 8.105, 5.958, 8.416Å 124°0'. The coeffs. of expansion along the major and minor axes of the mol. are 73.8 and 80.5, normal to the plane of the mol. 143.7 (all × 10⁻⁶). The av. values for the principal coeffs. of expansion are a_1 = 212.8 ± 4.0, a_2 = 6.3 ± 0.4, a_3 = 8.15 or 5.1 ± 0.1 (all × 10⁻⁶) (for a_3 the value of 6.15 is given in the summary, the value 5.1 in the body of the article). a_2 coincides with axis b, a_1 forms an angle of 44°10' with axis a.   R. F. Myers

PA 5b no 612 8798 (53)

KITAY - KILGRIY, B.I.

Crystal structure of Iodoform. T. L. Khotsyanova, A. I.
Kitaigorodskii, and Yu. T. Struchkov (Inst. of Org. Chem.,
Acad. Sci. U.S.S.R., Moscow). Zhur. Fiz. Khim. 27,
647-60(1953); cf. C.A. 47, 7854.—The crystal structure
of CHI_3 was detd. by x-ray diffraction. The valence angle
of CHI_3 was detd. by x-ray diffraction. The valence angle
I-C-I is 109 ± 3°. The bond length C-I is 2.18 ± 0.06 Å.,
0.06 Å. more than the value found by Bastiansen by elec-
tron diffraction. The distance between I atoms within the
mol. is 3.06 Å. The spatial arrangement of the mols. is de-
scribed and discussed. J. W. Lewisberg, Jr.

KITAY GORODSKIY, A. I.

5

U S S R .

548.736.1

401R. The crystal structure of iodine. A. I.
KITAYGORODSKII, T. L. KHOTSYANOVA AND YU. T.
STRUCHKOV, *Zh. fiz. Khim.*, 27, No. 6, 780-1 (1953).

In Russian.

The crystal structure of iodine has been redeter-
mined with results substantially in agreement with
earlier work. Atoms lie in (*f*) positions in the space
group Cmca with (*z*, *x*) parameters (0·149, 0·115,).
The 121 observed reflexions were corrected for
absorption and used to give a Patterson section at
y = 0. The molecular I-I distance was found to be
2·68 ± 0·01 Å, intralayer distances to be 3·56 and
4·04, and I-I distances between layers 4·35 and
4·38 Å. The form of the molecule is shown in a
diagram.

A. L. MACKAY

KITAYGORODSKIY, A.I.

Chemical Abst.
Vol. 48 No. 6
Mar. 25, 1954
General and Physical Chemistry

KITAYGORODSKIY, A I

U S S R

Crystal structure of tetraiodoethylene. T. L. Khotsyanova, A. I. Kitaigorodskii, and Yu. T. Struchkov (Inst. Org. Chem., Acad. Sci. U.S.S.R., Moscow). *Zhur. Fiz. Khim.* 27, 1331-13(1953); cf. C.A. 47, 7851f, 49, 2145g.— The cryst. structure of C_2I_4 was detd. by x-ray diffraction. The parameters of the monoclinic unit cell (a, b, c, and β) are 15.10 ± 0.05, 4.15 ± 0.02, 13.00 ± 0.04 A., and $106 \pm 1°$, resp. The unit cell has 4 mols.; the exptl. d. is 3.68. The space group is C_{2h}^5, $P2_1/c$. Within the mol. the distances C to C, C to I, and I to I (calcd. by means of a 3-dimensional electronic. phot.) are 1.34, 2.15, and 3.64 A., resp., and the angles I-C-I and I-C-C are 115°30' and 122°15', resp. The internal. radii of I and C are 2.0 and 3.85 A., resp. Coordinates of the atoms in the lattice are tabulated; the arrangement of the mols. in the crystal is discussed with illustrations.   J. W. Loveberg, Jr.

KITAYGORODSKIY, A.I.

USSR.

The method of röntgenographic analysis used in the study of the crystal structure of tetraiodoethylene. A. I. Kitaygorodskii, T. L. Khotsyanova, and Yu. T. Struchkov. Inst. Org. Chem., Acad. Sci. U.S.S.R., Moscow. *Izvest. Akad. Nauk. S.S.S.R., Otdel. Khim. Nauk.* 27, 1950-1950(1951)(in Russ.) A math. discussion. An objective method is proposed for the conversion of the results of relative measurements of F_{hkl} and F_{hkl} to abs. units and the calcn. of the mean f-curve. The validity of the at.-factor formula $f = ke^{-bs^2}$, where k and b are consts. and $s = 4\pi \sin\theta/\lambda$ is shown. Meths. are given for detg. the coordinates of atoms along one axis if the remaining coördinates are known, and for detg. the coördinates of max. in 2- and 3-dimensional series. Formulas for the probable error of detn. of electron d. are given and applied to exptl. data (l.c.). The detn. of light atoms in the presence of heavy ones is discussed.   J. W. L. K.

KOSTIN, A. I.

Low temperature investigation of the structure of aromatic compounds. II. Anisotropy of thermal expansion of nitracene. [by] M. Kostin and A. I. Kitaigorodskii.

The results of thermal expansion of anthracene were obtained ... the ellipsoid of expansion, and α_2 is the one along the minor axis. The direction of ... molecules with the crystallographic ... b, whereas that of ... forms an angle of 13° with ...

The coeffs of expansion for the axes of the unit cell are ...

KITAYGORODSKIY, A. I.

Chemical Abstracts
May 25, 1954
General and Physical
Chemistry

Crystal structure of products of addition of coumarin and mercuric chloride and bromide. Yu. T. Strychkov, A. I. Kitaygorodskii, and T. L. Khotsyanova. Doklady Akad. Nauk S.S.S.R. 91, 675 K(1953). — X-ray analysis of coumarin-HgCl₂ (I) and coumarin-HgBr₂ (II) addn. compds. was made. Both are isomorphous with space group P2₁/a on monoclinic syngony. There are 4 mols. per unit cell, whose dimensions are: I a 23.63 A., b 11.37, c 4.03, β 97°40', V 1004 cu. A.; II 24.01, 11.51, 4.10, 97°30', 1108 cu. A. The products are not added at the double bond of coumarin. The shortest Hg-Cl distance in a crystal of I is 3.3 A., and the products I and II are mol. compls. like RC.O...HgX₂. Cl atoms are at equal distance (2.33 A.) from Hg, with 171° angle. The Hg-O₂ distance is 2.38 A. The mols. are closely packed on the c axis, forming a twinned ribbon of octahedral Cl₂Hg₂O units. The following interat. distances are abnormal: C—O

(C in the 2 position) is slightly shortened; C=O is lengthened. Probable dispersitions are shown on diagrams. In II the shortening of Hg—O is Å (2.73 A.).   G. M. K.

KITAYGORODSKIY, Aleksandr Isaakovich, doktor fiziko-matematicheskikh nauk,
professor; LESHKOVTSEV, V.A., redaktor; KIPNIS, S.Ye., redaktor;
DMITRIYEVA, R.V., tekhnicheskiy redaktor.

[Physical principles of atomic energy] Fizicheskie osnovy iadernoi
energetiki. Moskva, Izd-vo "Znanie," 1954. 38 p. (Vsesoiuznoe ob-
shchestvo po rasprostraneniiu politicheskikh i nauchnykh znanii,
Ser. 3, no.57)   (MLRA 7:12)
        (Atomic energy)

KITAYGORODSKIY, A.I.; VOL'KENSHTEYN, M.V., redaktor; BELOVA, V.I.,
      redaktor; ASTAF'YEVA, O.A., tekhnicheskiy redaktor.

      [Order and confusion in the world of atoms] Poriadok i bes-
      poriadok v mire atomov. Moskva, Izd-vo Akad. nauk SSSR,
      1954. 69 p.   (MLRA 7:12)
              (Atoms) (Crystallography)

KITAYGORODSKIY, Aleksandr Isaakovich; MEZENTSEV, Vladimir Andreyevich;
KRIVOSHEYA, A.S., redaktor; ATAMASHKO, V.F., tekhnicheskiy redaktor.

[Atoms and molecules] Atom i molekula. Pereklad s rosiis'koho
vydannia. Kyiv, Dersh.uchbovo-pedahoh.vyd-vo "Radians'ka shkola,"
1954, 83 p. (Microfilm)   (MLRA 8;2)
        (Atomic theory)

KITATGORODSKIY, A.I.

"Theory of the Determination of Indicators of Structural Amplitudes," by
A.I. Kitaygorodskiy, pp. 27-41

SO: Works of the Inst. of Crystallography, Issue #10, (Reports submitted
at the 3rd International Congress of Crystallography; published by
the Acad Sci USSR, Moscow, 1954)

KITAYGORODSKII, A. (Prof.) (Dr. Physicomathematical Sci.)

"Atomic Energy," a 3-page article discusses in general the chemistry of the atomic nucleus, including nuclear reaction of uranium isotopes 235, in some detail, and 238 briefly; a nuclear reacter with a graphite moderator in detail, and with heavy water briefly.
Kryl'ya Rodiny, No 5, pp 18,19,20, May 1954

KITARYGORODSKIY, A.I., professor, doktor fisiko-matematicheskikh nauk
(Moscow)

Nuclear power engineering. Fis.v shkole 14 no.6:3-14 N-D '54.
        (Nuclear reactors)   (MLRA 7:12)

KITAYGORODSKIY, A. I.

USSR/ Physics - Analysis methods

Card 1/1   Pub. 13 - 9/62

Authors   :   Kitaygorodskiy, A. I.

Title   :   Elastic constants and the configuration of a molecule

Periodical   :   Izv. AN SSSR. Ser. fiz. 18/6, 664-665, Nov-Dec 1954

Abstract   :   A brief survey is given showing how the spectral and x-ray structural analysis methods make it possible to determine the configuration of molecules. X-ray structural analysis determines the structure and configuration of the molecule and the elasticity constants of valent angles are established spectroscopically. If it is assumed that the intermolecular forces vary linearly with the deformation of the atoms then each atom can be individually characterized by the compressibility coefficient.

Institution :   Acad. of Sc., USSR, Inst. of Elementorganic Compounds

Submitted   :   .....

KITAYGORODSKII A I.

Kitaigorodskii, A. I.   The theory of the statistical method of structure analysis.   Dokl. Akad. Nauk SSSR (N.S.) 94, 225-228 (1954).   (Russian)

$1 - F/\bar{n}$

KITAYGORODSKIY, Aleksandr Isaakovich

[Crystals] Kristally. Izd.3. Moskva, Gos.izd-vo tekhn.-teoret.
lit-ry, 1955. 62 p. (Nauchno-populiarnaia biblioteka, no.19)

(MIRA 13:3)

(Crystallography)

KITAYGORODSKIY, A.I., professor; KAIZR, Ya.M., redaktor; MIKHAYLOV, V.A., kandidat fiziko-matematicheskikh nauk, inzhener-podpolkovnik; SOROKIN, V.V., tekhnicheskiy redaktor.

[Structure of matter and its energy] Stroenie veshchestva i ego energiia. Moskva, Voen. izd-vo Ministerstva oborony SSSR, 1955. 125 p.
(MIRA 8:4)
(Matter) (Atomic energy)

KITAYGORODSKIY, A.I.; BOKIY, G.B., professor, otvetstvennyy redaktor;
STRUCHKOV, Iu.T., redaktor; ENVRAYEVA, N.A., tekhnicheskiy re-
daktor

[Organic crystallochemistry] Organicheskaia kristallokhimiia. Mo-
skva, Izd-vo Akademii nauk SSSR, 1955. 558 p.   (MIRA 8:7)
     (Crystallochemistry)

KITAYGORODSKIY, A.I.

USSR/ Chemistry - Physical chemistry

Card 1/1   Pub. 147 - 17/21

Authors   : Kozhin, V. M., and Kitaygorodskiy, A. I.

Title   : Low temperature investigation of the structure of aromatic compounds.
             Part 3. Crystalline and molecular structure of naphthalin

Periodical : Zhur. fiz. khim. 29/1, 1897-1908, Oct 1955

Abstract   : A complete structural investigation of naphthalin was made at -195° C.
             Three-dimensional series were formulated and the coordinates of atoms
             and atomic functions were compared for temperatures of -195° and -20° C.
             An analysis of the interatomic spaces showed that the contration in the
             nucleus is due to the changes in the spaces between various molecules.
             Equalization of the intermolecular radii was observed during temperature
             drops. Five references: 4 USSR and 1 USA (1946-1953). Tables; diagrams.

Institution : Acad. of Sc., USSR, Inst. of Organoelemental Compounds, Moscow

Submitted   : April 6, 1955

USSR/ Chemistry - Physical chemistry

Card 1/1   Pub. 147 - 14/22

Authors   : Kozhin, V. M., and Kitaygorodskiy, A. I.

Title   : Low temperature investigation of the structure of aromatic compounds.
             Part 4. The anisotropy of thermal expansion in benzene

Periodical : Zhur. fiz. khim. 29/11, 2074-2075, Nov 55

Abstract   : The anisotropy of thermal expansion in benzene was measured on benzene
             monocrystals by means of x-ray structural analysis. The dimensions of an
             elementary nucleus for temperatures of -20 and -195°C were established.
             The mean thermal expansion coefficients in the direction of the main ther-
             mal deformation axes of the benzene crystal were determined. It was found
             that an increase in the molecule per one benzene ring is connected with a
             constant ratio of mean volumetric values of the expansion coefficients.
             Six references: 2 USSR, 2 USA, 1 Germ. and 1 Ital. (1924-1954). Drawing.

Institution : Acad. of Sc., USSR, Inst. of Organoelemental Compounds, Moscow

Submitted   : April 6, 1955

KITAYGORODSKIY, A. I.

USSR/ Chemistry - Crystallography

Card 1/1   Pub. 22 - 19/51

Authors   :   Kitaygorodskiy, A. I.

Title   :   The theory of determining signs of structural amplitudes

Periodical :   Dok. AN SSSR 101/1, 73-76, Mar 1, 1955

Abstract   :   Experiments showed that the newly prepared theory of determining
                signs of structural amplitudes is based on the analysis of a certain
                expression. It is explained that the absolute value of structural
                amplitudes F can be found by studying the centro-symmetrical crystal
                by means of the x-ray analysis method. A formula is presented for
                the calculation of single structural amplitudes. Differences in the
                sign can be seen only in the case of faint reflections at a considerable
                deviation of the atoms from the parallel line. The numerical values
                of some structural amplitudes were found to be independent from each
                other. Eight references; 1 USSR and 7 English (1949-1954).

Institution :   ...of Sci., USSR, Institute... of ... Organic Compounds

Presented by :   Academician G. V. Byalon, November 6, 1954

KITAYGORODSKIY, A. I.

USSR/ Chemistry – Crystallography

Card 1/1   Pub. 22 – 26/62

Authors   : Kitaygorodskiy, A. I.

Title   : New method of direct structural analysis of crystals

Periodical : Dok. AN SSSR 102/3, 519 – 520, May 21, 1955

Abstract   : A new method of direct structural analysis of crystals is briefly described.
            The method makes it possible to establish the arrangement of atoms in the
            elementary nucleus of the crystal without any hypotheses regarding the
            structure of the crystal and without the need of structural models. Some
            results obtained by the new method are listed. One USSR reference (1955).

Institution : Acad. of Sc., USSR, Inst. of Elementorganic Compounds

Presented by: Academician N. V. Belov, February 15, 1955

Kitaygorodskiy, A. I.

USSR/Solid State Physics - Structural Crystallography, E-3

Abst Journal: Referat Zhur - Fizika, No 12, 1956, 34585

Author: Kitaygorodskiy, A. I.

Institution: Institute of Elementary Organic Compounds, Academy of Sciences USSR

Title: Theory of Connection Between Structural Amplitudes

Original Periodical: Dokl. AN SSSR, 1955, 105, No 3, 482-484

Abstract: General relationships are obtained between individual structural ampli-
tudes. To derive the relationship, one introduces a linearly-independent vector of
the type   The scalar products of the vectors $G_p G_q^s$ is

$$G_p = \sum_{j=1}^{N} e_j n_j^{1/2} \exp 2\pi i H_p r_j$$

equal to the single structural amplitude of the H_p - H_q lattice point of the inverse
lattice. Assuming that the vectors G_1, G_2, G_3...G_{m-1} are fixed and that the values
of the structural amplitudes $F_{1,m}$, $F_{2,m}$,...$F_{m-2,m}$ are known, or what is the same,
the cosines of the angles between the vectors G_1 and G_m; G_2 and G_m; ..., G_{m-2} and
G_m are known, it is possible to explain the limitations that are imposed thereby on
the position of the vector G_m. The relationship $F_{m,m-1} = A + B \cos \varphi$, is established,

USSR/Solid State Physics - Structural Crystallography, E-3

Abst Journal: Referat Zhur - Fizika, No 12, 1956, 34585

Author: Kitaygorodskiy, A. I.

Institution: Institute of Elementary Organic Compounds, Academy of Sciences USSR

Title: Theory of Connection Between Structural Amplitudes

Original Periodical: Dokl. AN SSSR, 1955, 105, No 3, 482-484

Abstract: where A and B are expressed in the terms of all the remaining specified F_{pq}. This relationship appears to be the most general. The known inequalities, relating the structural amplitudes, and also all the probability relationships, should follow from this relationship.

KITAYGORODSKIY, Aleksandr Isaakovich; GUROV, K.P., redaktor; KUZNETSOVA, Ye.B., redaktor; TUMARKINA, V.A., tekhnicheskiy redaktor

[Order and disorder in the world of the atoms] Poriadok i besporiadok v mire atomov. Izd. 2-oe, perer. i dop. Moskva, Gos. izd-vo tekhniko-teoret. lit-ry, 1956. 138 p.   (MLRA 10:2)
        (Atoms)

KITAYGORODSKIY A.I.

dup.

Category : USSR/Solid State Physics – Structural Crystallography   E-3

Abs Jour : Ref Zhur – Fizike, No 3, 1957, No 6508

Author   : Kitaygorodskiy, A.I.
Inst   : Institute of Elementary Organic Compounds, Academy of
           Sciences, USSR.
Title   : Kristallografiye, 1956, 1, No 1, 14-16

Abstract : On the basis of the theory of the connection between the
           structural amplitudes, developed by the author, plots are
           prepared for the determination of the reliably positive
           structural products $F_H^2 x^2 F_{K-H}$. Using the author's formula
           for the probability of the positive sign of the structural
           product, $\omega_+ = 1/(1 + \zeta)$, where

$$\zeta = \sqrt{\frac{1 - \bar{F}_H^2 - \bar{F}_K^2 - \bar{F}_{K\cdot H}^2 - 2|\bar{F}_H \bar{F}_K \bar{F}_{K\cdot H}|}{1 - \bar{F}_H^2 - \bar{F}_K^2 - \bar{F}_{K\cdot H}^2 + 2|\bar{F}_H \bar{F}_K \bar{F}_{K\cdot H}|}}$$

           curves are plotted for the probability of the positive sign
           for structural products of different magnitude and of dif-
           ferent dependence of $x = F_H|\cdot|F_K|$. It is established that

Card   : 1/2

KITAYGORODSKIY, A. I.

USSR/ Chemistry - Molecular compounds

Card   1/1   Pub. 40 - 20/25

Authors   : Kolesnikov, G. S.; Korshak, V. V.; Andreyeva, M. A.; and Kitaygorodskiy, A. I.

Title   : High molecular compounds. Part 90. Polycondensation of 1,2-dichloroethane with tetralin

Periodical : Izv. AN SSSR. Otd. khim. nauk 1, 114-119, Jan 1956

Abstract   : The polycondensation of 1,2-dichloroethane with tetralin was investigated in the presence of aluminum chloride and the basic laws governing this polycondensation process were established. On the basis of x-ray analysis it was determined that 1,2-di-(beta-tetralyl) ethane is the product obtained during the initial polycondensation stages. The formation of three-dimensional polycondensation products was observed in spite of the fact that the potential function of tetralin is only 4. The effect of benzene-solution concentrations of polytetralylenethyl on the polymer molecule association is discussed. Seven references: 5 USSR and 2 Germ. (1921-1955). Tables; graph.

Institution : Acad. of Sc., USSR, Inst. of Organoelemental Compounds

Submitted   : November 18, 1954

KITAYGORODSKIY, A.I., professor, dokter fiziko-matematicheskikh nauk.

Interesting facts on important things ("Time and its measurement."
F.S.Zavel'skii. Reviewed by A.I.Kitaigorodskii). Nauka i zhizn' 23
no.9:60 '56. (Time measurements)   (MLRA 9:10)

KITAYGORODSKIY, A.I., professor (Moskva)

In the world of physics ("Universe and atom." Y. Mesentsev.
Reviewed by A.I. Kitaigorodskii. Priroda 45 no.2:119-120 F '56.
(Atoms)   (MLRA 9:5)

KITAYGORODSKIY, A. Y.

Institute of Elemento-Organic Compounds, Moscow-"Theorie de Correlation entre les Facteurs de Structure et les Methodes Directes de l'Analyse de Structure" (Section 2-13) " Sure les Cristaux Mixtes de Composents Organiques" (Section 7-1); L'Empaquetage de Molecules Longues" (Section 7-19) papers submitted at the General Assembly and International Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

C-3,800,189

KITAYGORODSKIY, A. Y., KHOTSYANOVA, T. L., and STRUCHKOV, G. T.

Institute of Elemento-Organic Compounds, Moscow: "The Crystal Structure of Some Tropylium Salts" (Section 7-11) a paper submitted at the General Assembly and International Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

C-3,800,189

SHAPIRO, A. L.

"X-ray investigation of linear polyethers," a paper presented at the 1st Congress on the Chemistry and Physics of High Polymers, 28 Jan.-2 Feb 57, Moscow. Research Inst. for Organic Chemistry, AN USSR.

B-3,064,305

Kitaygordskiy, A.I.

NUCLEAR TECHNOLOGY AND APPLICATIONS: POPULAR SURVEYS

Structure of Matter and Its Energy, by Professor A. I. Kitaygorodskiy.
Second, corrected and supplemented edition; Moscow: Military Publishing
House of the Ministry of Defense USSR, 1957. 200 pages, 5 x 8 inches.

A popular book, apparently intended for people untrained in chemistry
and physics. The table of contents follows: "Introduction;" "Structure
of matter;" "Convenient measurement units;" "Atoms;" "Molecules;" "Var-
ious types of atoms of a chemical element;" "Decaying atoms;" "Three states
of matter;" "Crystals;" "Invisible movements;" "Measurement of interac-
tomic distances;" "Structure visible to the aided eye;" "Energy of matter;"
"Mechanical energy and heat;" "Transformations of molecules;" "Chemical
energy;" "Nuclear energy: collisions of atomic nuclei; artificial atoms;
is it possible to obtain heat during nuclear transformations? nuclear
fuel; operating principle of the atom bomb; operating principle of the
nuclear reactor; constructions of nuclear reactors; soviet nuclear re-
actors; breeder reactors; problem of heat removal; protection against

Card: 1/2

KITAYGORODSKIY, Aleksandr Isaakovich; VAYNSHTEYN, B.K., doktor fiziko-matem.nauk,
otvetstvennyy red.; SHMIDT, V.V., red.izdatel'stva; ASTAF'YEVA,G.A,tekhn.red.

[A theory of structural analysis] Teoriia strukturnogo analiza.
Moskva, Izd-vo Akad.nauk SSSR, 1957. 283 p.   (MIRA 10:12)
                    (Crystallography, Mathematical)

KITAYGORODSKIY, A.I.

The structure of high polymers. Usp. khim. i tekh. polim. no.2:191-
201 '57.   (MIRA 11:1)

(Polymers)   (Molecular structure)

70-3-5/20

AUTHOR: Kitaygorodskiy, A.I.

TITLE: Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure. (Teoriya svyazi strukturnykh amplitud i metody pryamogo analiza struktury kristallov)

PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol. 2, No.3, pp. 352 - 357 (U.S.S.R.)

ABSTRACT: The law of predominat positivity of $F_H F_K F_{H+K}$ has been elucidated, a new method of its use for direct structure analysis being proposed. It has been demonstrated that statistical theories are of secondary importance both for proving and applying this law.

A very interesting rule can be deduced experimentally, namely: the structural product $X_{HK} = F_H F_K F_{H+K}$ is positive in most cases; the larger the absolute value of the structural product the larger will be the positive part of X_{HK}. The first definition of this law was given by this author in 1953 (4); he has shown that the law can be deduced on the assumption of a uniform distribution of the arguments of trig-onometric functions which enter into the formulae of the structural factors. With this assumption, it is possible to

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Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure. (Cont.)

determine the function of probability of the value X_{HK} and thus to show that it has a maximum value in the positive range. In the mentioned earlier work, it was shown that the possibility of a positive sign of the structural product can be expressed by:

$$W_+ = (1 + \exp [-2NX_{HK}])^{-1},$$

where N is the effective number of atoms on the lattice. Such a theory can be referred to as a statistical theory and it enables explanation of the predominance of the positive value of X_{HK} and the fact that statistical ideas should be the basis of direct methods of structural analysis. By a more detailed study, the author shows that this view is erroneous; statistical theories have a predominance rule only in the case of small X_{HK} values. For large X_{HK} values (and only large values have any practical interest) the law of predominance of the positive value of X_{HK} has a completely different and

Card 2/7

Theory of the correlation between the structural factors and the methods of direct analysis of the crystal structure. (Cont.)

more accurate explanation which does not presuppose any assumption or hypothesis. Particularly, the law of predominance is correct in the case in which all the atoms are in special positions and when the arguments (HP) can assume any small number of discreet values. In earlier works, the author has shown that the structural product is definitely positive if $|x_{HK}| > 1/8$. However, in the case of less rigid conditions, a non-statistical approach exists (i.e. for which there is no correlation between the character of the distribution of the atom co-ordinate in the lattice) which leads to a law of predominance of positive x_{HK} values. The most general correlation between structural factors is achieved if the determinant D_m has a positive value:

$$D_m = \begin{vmatrix} 1 & \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ F_H & 1 & \cdots\cdots\cdots\cdots\cdots\cdots \\ F_K & F_{K-H} & 1 & \cdots\cdots\cdots \\ F_L & F_{L-H} & F_{L-K} & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{vmatrix} > 0.$$

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70-3-5/20

Theory of the correlation between the structural factors and
the methods of direct analysis of the crystal structure.
(Cont.)

This determinant can be written in the form of a well-known
series and we thus obtain:

$$1 - \sum_H P^2_H + \sum_{H,K} P_H P_K P_{H+K} - \ldots > 0.$$

The here written terms are the most important of the sum. It is
obvious that the positive value of the sum can be obtained only
if the largest part of the structural products are positive.
This formula shows that all the structural products, without
exception, will be positive if the values of P composing the
determinant exceed a certain limit δ. Thus, the direct method
of determination of the signs of the structural factors is based
on the property of the determinant D_m and not on the ideas of
statistical distribution of the atomic co-ordinates in the
lattice. The predominance of the positive values of large
structural products does not correspond to any statistical theory
whatever. If the structural product is not an absolute posi-
tive value the question of probability of its positive sign can
be discussed..Inaccurate formulation and ignoring the absolute
correlations between the factors has led various authors to

Card 4/7

70-3-5/20

Theory of the correlation between the structural factors and
the methods of direct analysis of the crystal structure.
(Cont.)

calculating the probability density of the structural product
instead of calculating the probability of the structure for
which the structural product has a given value. The expressions
for the probability of the sign being positive for X_{HK} deduced
in previous work does not indicate the existence of any critical
value of X when the probability is reduced to one. The
correct expression for the probability of the positive sign of
the structural product is $W_+ = 1/(1 + \varepsilon)$, where

$$\varepsilon = \sqrt{\frac{1 - P^2_H - P^2_K - P^2_{K+H} - 2P_H P_K P_{K+H}}{1 - P^2_H - P^2_K - P^2_{K+H} + 2P_H P_K P_{K+H}}}$$

$$\times \exp\left[- 2N \cdot P_H P_K P_{K+H}\right].$$

The author believes that formulae of statistical origin are
of secondary importance. The direct methods which permit finding
Card 5/7 the signs of the structural factors are effective only in the
case where a large number of structural products have definitely

Theory of the correlation between the structural factors and
the methods of direct analysis of the crystal structure.
(Cont.)

a positive sign. The good results obtained by the direct
method are not at all linked with statistical theories. The
author believes that work with direct methods should be effec-
ted by composition of all types of D_m determinants. The
correct signs of the structural factors should not give a neg-
ative value to any determinant. It is shown that the rule:
$X_{HK} > 0$ if $|X_{HK}| > -1/8$ can be extended to determinants of
any order. If the determinant of the order m is composed
of F for which $|F| > 0_m$, all the structural products which
do not enter into the determinant are definitely positive.
The magnitudes of Φ_m decrease with increasing m. Analysis
of the determinants of high orders permits judgment of the
positivity of a structural product one hundred times smaller
than 1/8. The author believes that the method which permits
direct determination of the signs of the structural factors
will play an important role in X-ray structural analysis.
However, for this purpose, the use of computers is indispensable.

Card 6/7

A I T A Y O G K C D U (Y, A I

70-4-2/16

AUTHOR: Kitaygorodskiy, A.I.

TITLE: Ideas relating to organic crystallo-chemistry (Idei organicheskoy kristallokhimii)

PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol.2, No.4, pp. 456 - 465 (U.S.S.R.)

ABSTRACT: The thermodynamical aspect of the theory of close packing of molecules in crystals is discussed and new applications are considered of the theory for the purpose of deriving the possible structures of paraffin crystals, as well as establishing the conditions involved in the formation of solid solutions. The ideas of the author relating to the symmetry and the density of packing of molecules in a crystalline system enabled formulation of the following rules of formation of maximum organic crystals: 1) the solutions of "interclusion" can form only if the volumes of the molecules are in the ratio (8 to 10): 1; 2) substitution solutions always exist when the configurations of the molecules forming the mixture are sufficiently near to each other; 3) mixed crystals can form at any ratios under the above mentioned conditions only if the packing symmetry of the molecules (spatial group and number of molecules in the lattice) is equal for the individual components. Molecules which possess a centre of symmetry maintain it

Card 1/3

70-4-2/16

Ideas relating to organic crystallo-chemistry. (Cont.)

inside the crystal. From this and from the last mentioned rule, it can be seen that molecules like those of naphthalene or anthracene cannot constitute a continuous series of solutions with mono-derivatives. Most of the data concerning continuous series disagree with the above mentioned condition and therefore one must conclude that these data are erroneous. For verifying the above mentioned rules, the author studied the systems dibenzyl-stilbene, phenanthrene-anthracene and anthracene. Data of published work indicate that these components form a continuous series of solutions. The above mentioned third rule indicates, however, that such continuous solutions cannot exist. In the three cases mentioned, the author obtained perfect crystals of mixtures of each composition; the diffraction diagrams established by means of Weissenberg goniometer have shown that the here mentioned rule is correct and that the previous experimental results were erroneous. The studied systems have diagrams of state with a eutectic and a pereutectic. Substitution of the molecules is absolutely irregular. The entry of one molecule of a different substance in the crystal is controlled solely by the law of close packing. This indicates that the foreign molecule chooses such a position in which the intra-molecular distances differ as slightly as

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Card 3/3

AUTHOR: Kitaygorodskiy, A.I.

TITLE: The Packing of Chain Molecules (Upakovka tsepochechnykh molekul) II. Layers of Paraffin Molecules (II. Sloi molekul parafinov)

ABSTRACT: On the basis of the theory of the close-packing of molecules (see Organicheskaya Kristallokhimiya, 1955 by A.I. Kitaygorodskiy) the possible symmetries and dimensions of layers of paraffin molecules are deduced. Three pseudocells are first distinguished R-orthorhombic with $a_0 = 4.96$, $b_0 = 7.42$ and $c_0 = 2.54$ A; M- monoclinic with $a_0 = 4.2$, $b_0 = 4.4$, $c_0 = 2.54$ A and $\gamma = 111^0$; T-triclinic with $a_0 = 4.3$, $b_0 = 4.8$, $c_0 = 2.54$ A and $\alpha = 90^0$, $\beta = 108^0$, $\gamma = 107^0$. m is a whole number, $c_0 = 2.54$ A is the distance between two methylene groups so that the identity distance parallel to c_0 is mc_0 A. m is the displacement of the molecule parallel to the a-axis and n parallel to the b-axis. The two-dimensional layer cell is determined by the pseudo-cell and by m and n. Each pair of numbers m and n give

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The Packing of Chain Molecules. II.   Layers of Paraffin Molecules.

four layers: m, n; $\bar{m}$, $\bar{n}$; $\bar{m}$, n; m, $\bar{n}$.   The possible layers
are tabulated: T-pseudocell - the ab plane of the layer
coincides with the $a_o b_o$ plane of the pseudocell and the
symbols are T(1/2, 0) and T(-1/2, 0). Each molecule has 6
neighbours. M-pseudocell - besides the rectangular layer
M(0, 0) there are oblique layers M(1, 0), M(-1, 0), M(0, 1)
and M(0, -1). R-pseudocell - besides the rectangular layer
R(0, 0) there are oblique layers R(0, 1), R(0, -1); R(1,0)
and R(-1, 0) and four layers with m and n equal R(1, 1),
R(1, -1), R(-1, 1) and R(-1, -1). The geometrical parameters
of these layers are tabulated (cell edges and angles). The
symmetry of the layers is determined not only by the geometrical
parameters but also by the symmetry of the particular molecules.
If the paraffin chain has an even number of C atoms, then its
symmetry is 2/m if an odd number, then mm. The various
combinations of symmetry are tabulated diagrammatically.
There are 3 figures, 1 table and 4 references, 1 of which is
Slavic.

ASSOCIATION: Institute of Elemental-organic Compounds.
Card 2/3   (Institut Elementoorganicheskikh soyedineniy)

70-5-13/31

. . cking of Chain Molecules.   II. Layers of Paraffin Molecules.

. . . ED: May 15, 1957.

AVAILABLE: Library of Congress

. . 5/5

KITAYGORODSKIY, A.I.

AUTHOR: None Given.

TITLE: General Meeting of the Department for Chemical
              Sciences of the AN USSR Held in May 30-31, and
              June 28, 1957 (Obshchiye sobraniya Otdeleniya
              khimicheskikh nauk Akademii nauk SSSR 30-31 maya i 28
              iyunya 1957 g).

PERIODICAL: Izvestiya AN SSSR, Otdel. Khim. Nauk, 1957, Nr 11,
              pp. 1416-1419 (USSR)

ABSTRACT: Chairman: Member of the Academy A. P. Vinogradov.
              Lectures: A. N. Terenin, Member of the Academy.
              "Spectroscopy of the Molecular Compounds with Metal Halides."
              V. N. Filimonov, the student D. Borsovyy and Sh. Sh. Raskin
              helped the author in his work.
              S. Z. Roginskiy, corresponding Member of the Academy,
              B. V. Nekrasov, corresponding Member of the Academy,
              N. D. Sokolov, Doctor of chemical sciences, M. M. Shemyakin,
              corresponding Member of the Academy, A. I. Kitaygorodskiy,
              Doctor of physico-mathematical sciences, A. P. Vinogradov,
              Member of the Academy, took part in the discussion.
              B. P. Nikol'skiy, corresponding Member of the Academy of

Card 1/3

KITAYGORODSKIY, A.I., doktor fiziko-matematicheskikh nauk.

First book on the subject ("Structural electronography" by B.K.
Vainshtein. Reviewed by A.I. Kitaigorodskii). Vest.AN SSSR 27 no.4:
136-138 Ap '57.   (MLRA 10:5)
        (Electron diffraction examination)
        (Vainshtein, B.K.)

ABSTRACT   The attempt was made to determine the correlation between the
            amount of solubility and the dimensions of the cavities and bul-
            ges formed on the occasion of mixing. Dissolution by penetration
            is possible only in the rarest of cases in organic systems. The
            packing coefficients of the organic molecules in the crystal are
            within range of from 0,6 to 0,8. This means that in organic cry-
            stals only small cavities are possible. These cavities have a to-
            tal volume of 10% of the molecular volume. Thus, solid solutions
            can be formed when A penetrates into B only if the molecules of A
            are about ten times smaller, with respect to volume, than those of
            B. It stands to reason that not only the volume but also the sha-
            pe of the cavities is of importance. If the molecules of A and B
            are more or less equal with respect to size and shape, the mole-
            cules of A are able to replace those of B in the crystal. The sym-
            metry of molecular distribution in the crystal changes abruptly
            as soon as the first molecules of A enter the solution,if the mo-
Card 1/2   lecules of B are not asymmetric, but if those of A are asymmetric

Card 2/2

KITAYGORODSKIY, A. I.

"Some Physical Problems of Organic Crystals."

report presented at the Conf. on Mechanical Porperties of Non-Metallic
Solids, Leningrad, USSR, 19-26 May 1958.

Inst. of Elemento-Organic Compounds, Moscow.

HALPERIN, A. I., A. S. AKHMANOV, L. V. ROKHLINA, M. V. VOL'KENSHTEIN

"Defective Crystallic States."

report presented at the Conference on Investigation of Mechanical Properties of Non-Metals, by the Intl. Society of Pure and Applied Physics and the AS USSR, at Leningrad, 19-24 May 1958.
(Vest. Ak Nauk SSSR, 1958, no. 9, pp. 109-111)

KITAYGORODGKIY, A. I.

A. I. Kitaygorodskiy and Yu. T. Struchkov, "Conformations of Molecules of Sterically Stretch Benzene Polyderivatives."

report presented at the Symposium on Concepts of Conformation in Organic Chemistry which took place in Moscow at the IOKh AN SSSR (Institute of Organic Chemistry, AS USSR) from September 30 to October 2, 1958.

Izvestiya Akademii nauk SSSR, Otdeleniye khimicheskikh nauk, 1959, No. 3, 561-564.

5(3)   PHASE I BOOK EXPLOITATION   SOV/1405

Kitaygorodskiy, Aleksandr Isaakovich

Struktura polimerov (Structure of Polymers) Moscow, Izd-vo
"Znaniye," 1958. 28 p. (Series: Vsesoyuznoye obshchestvo
po rasprostraneniyu politicheskikh i nauchnykh znaniy.
Seriya VIII, 1958; vyp. II, no. 21) 48,000 copies printed.

Sponsoring Agency: Vsesoyuznoye obshchestvo po rasprostraneniyu
politicheskikh i nauchnykh znaniy.

Ed.: Faynboym, I.B.; Tech. Ed.: Berlov, A.P.

PURPOSE: This book is intended for persons engaged in textile
manufacturing, biological research, structural engineering or
any field where polymers or high-molecular compounds are of
interest.

Card 1/ 2

Structure of Polymers   SOV/1405

COVERAGE: The book explains the structure and mechanism of formation of high-molecular compounds as a basis for determining the properties of plastics and artificial fibers and the structure of proteins and other biologically important substances which may explain the biochemical and biological behavior of test subjects. Diagrams and drawings of bond distribution, atomic arrangements and crystal orientation are given. The following new theory of the structure of polymers by V.A. Kargin, A.I. Kitaygorodskiy and G.L. Slonimskiy is discussed: a polymeric subatance is thought to consist of non-entangling bundles of long-chain molecules, molecules of different length (weight) constituting the same bundle as if following each other. Other such molecules constitute neighboring chains, which maintain their position throughout the bundle. A bundle may shift its direction as a whole in patterned (regular) fashion. By this regular shifting, all molecules lie in the same plane.

CONTENTS:

Chemical Structure
The Structure of Molecules   3
The Structure of a Polymeric Substance   7
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AVAILABLE: Library of Congress

Card 2/2   TM/bj
                                            4-29-59

AUTHORS: Myasnikova, R.M. and Kitaygorodskiy, A.I.   70-3-2-5/26

TITLE: The Structures of Mixed Crystals of the System Acridine-Anthracene (Stroyeniye smeshannykh kristallov sistemy akridin-antratsen)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 160 - 166
(USSR).

ABSTRACT: The anthracene and acridine molecules are geometrically similar but owing to the presence of a nitrogen atom in the acridine molecule, their symmetries are mmm and $mm2$ respectively. It was earlier thought that a continuous range of solid solutions is formed but this is shown to be incorrect and that there are breaks at 4% and 28% anthracene. From 0- 4.6% anthracene needle crystals are formed; between 4.6 and 28.2% monocrystals were not formed and at greater concentrations plates were produced. The unit cell dimensions were: 100% acridine a.$\sin\beta$=16.35, b=18.51, c = 6.07 Å, packing coefficient k=0.713; 4.6% anthracene a.$\sin\beta$=17.08, b=19.60, c=6.08, k=0.644; 28.2% anthracene a=8.421, b=6.06, c=11.054, β=123°46', k=0.707; 100% anthracene a = 8.561, b=6.036, c=11.163, β=124°42', k=0.722. At the anthracene-rich end there are 2 molecules per unit cell and at the other end 8 molecules.

Card1/2

The Structures of Mixed Crystals of the System Acridine-Anthracene
70-3-2-5/26

There are 4 figures, 2 tables and 6 references, 3 of which are Soviet and 3 English.

ASSOCIATION: Institut elementoorganicheskikh soyedineniy AN SSR
               (Institute of Elemental-organic Compounds, Ac.Sc. USSR)

SUBMITTED: July 9, 1957

Card 2/2

KITAYGORODSKIY, A. I.

AUTHORS: Belov, N.V., Belyayev, L.M., Boky, G.B., Bronshtova, Ye.S.,
Vaynshteyn, B.K., Indenbom, V.L., Jurnakov, V.I., Kitaygorod-
skiy, A.I. and Pinsker, Z.V.

TITLE: The Fourth International Congress of Crystallography
(IV mezhdunarodnyy kongress kristallografov) (Montreal,
July 10-19, 1957)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 230 - 240
(USSR).

ABSTRACT: Outline of the scientific proceedings of the
conference.

Card 1/1

AUTHORS: Kitaygorodskiy, A.I., Mnyukh, Yu.V. and Nechitaylo, N.A.   70.3.3-7/36

TITLE:.   An Investigation of Solid Solutions of Certain n-paraffins
          (Issledovaniye tverdykh rastvorov nekotorykh n-parafinov)

ABSTRACT: X-ray and thermographic analysis of the binary systems
        formed from the paraffins with C_{18}, C_{19} and C_{20} were made.
        Regularities followed from the theory of close packing of
        molecules were established and an orthorhombic phase was found
        in C_{18} - C_{20}. In identical conditions the solubility of
        molecules wity longer chains is less than that of molecules
        with shorter chains. The theoretical conclusion on the impossi-
        bility of a continuous range of solid solutions in mixtures of
        odd and even paraffins was confirmed.
        X-ray powder photographs were taken at room temperature and
        at temperatures from -100 °C up to the melting points. It
        was found that in the systems C_{18} - C_{19} and C_{20} - C_{19} there
        was no continuous range of solid solutions. The C_{18} - C_{20}
        system also showed no continuous range of solid solutions
Card1/2 in spite of the isomorphism of the crystals $C_{18}H_{38}$ and

An Investigation of Solid Solutions of Certain n-paraffins   70-3-3-7/36

$C_{20}H_{42}$ which are tri-clinic with very similar dimensions.
The region from 8% C_{20} to 81% C_{20} was orthorhombic.
Phase diagrams of the systems $C_{12} - C_{13}$, $C_{13} - C_{14}$ and
$C_{14} - C_{15}$ are given. The increased solubility of shorter
molecules in a given solvent is explained by the lesser
disturbance to the structure caused by holes in the structure
compared to that caused by extra groups intruding.
There are 5 figures and 9 references, 6 of which are Soviet,
2 English and 1 French.

ASSOCIATION: Institut elementoorganicheskikh soyedineniy, Institut
              nefti (Institute of Elemental-organic Compounds. Oil
              Institute)

SUBMITTED: December 4, 1957.
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70-3-3-34/36

AUTHOR: Kitaygorodskiy, A.I.

TITLE: On the Impossibility of Distributing Centro-symmetrical
Molecules in Non-centrosymmetrical Groups (O nevozmozh-
nosti razmeshcheniya tsentrosimmetrichnykh molekul v
netsentrosimmetrichnykh gruppakh)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 391 - 392
(USSR)

ABSTRACT: A statement by Gerbstein and Schöning (Acta Crystallogr.,
Vol 10, p 657, 1957) that centrosymmetric molecules can form
crystals without a centre of symmetry is contested. Two cases
are examined: 1) The number of molecules is equal to the
multiplicity of the general position in the group. The group
$P2_1$ is used as an illustration, the contention being demon-
strated for this case. In the case 2) the number of molecules
is greater than the multiplicity of the general position and
not all molecules are identically situated. Here, centro-
symmetrical molecules must associate into non-centrosymmetrical
groups; this contradicts principles set out by Kitaygorodskiy
in his book "Organicheskaya kristallokhimiya". The four
examples which Gerbstein and Schöning quote are criticised as
being of definite space group but uncertain centrosymmetry of
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On the Impossibility of Distributing Centrosymmetrical Molecules in non-centrosymmetrical Groups

the molecules. For mercury ethyl mercaptan, only the positions of the heavy atoms were determined. Difluorenildene is more doubtful and steric hindrance may make the fluorene nucleus non-planar. In 4, 4'dinitrodiphenyl steric hindrances due to the ortho atoms of hydrogen disturb the planarity. 1,2,5,6-dibenzanthracene exists in two modifications, the α-modification being centrosymmetrical and the β assumed non-centred. This assumption is contested. The β is thought to be a cis-form and the α a trans-form.
There are 2 Soviet and 1 English references.

ASSOCIATION: Institut elementoorganicheskikh soyedineniy
                (Institute of Elemental - Organic Compounds)

SUBMITTED: December 27, 1957
Card 2/2

AUTHOR: Kitaygorodskiy, A. I., Doctor of Physical and Mathematical
               Sciences

TITLE: The Problem of the Structure of High-Molecular Substances
               (Problema stroyeniya vysokomolekulyarnykh veshchestv)

PERIODICAL: Vestnik Akademii nauk SSSR, 1958, Nr 6, pp. 35 - 42 (USSR)

SOV/30-58-6-4/45

ABSTRACT: Synthetic materials, synthetic fibers, cellulose, albuminous
               substances, give an idea of the place taken by high-molecular
               substances in modern engineering and biology. According to
               the author's opinion, the investigators face two tasks: the
               first consists in finding common rules governing the structure
               of such substances as linear polymeric compounds and globular
               albuminous substances; the second consists in the development
               of detailed methods of the structural characteristic of in-
               dividual substances. Only 2 classes of high-molecular com-
               pounds can at present be discussed from the general point of
               view - linear polymeric compounds, as well as globular pro-
               tein. Moreover, the author explains his proposal for the
Card 1/4   solution of the structural problem of linear polymeric com-

The Problem of the Structure of High-Molecular Substances   30V/30-58-6-4/45

pounds. This problem consists in the problems of the structur-
al investigation of both individual molecules and molecule-
-conglomerates. The structural investigation of the elements
of which the albumin molecules consist, ought to precede
the investigation of the albuminous structures. Concerning
the production of high-molecular materials with the proper-
ties required, the problems of reciprocal arrangement of the
molecules do not play a smaller part than the problems con-
nected with the structure of an individual molecule. The
author refers here to his previous work which he carried out
in collaboration with V. A. Kargin and G. L. Slonimskiy
(Ref 1). Regarding the problems of organic crystal chemistry,
the author refers to his previous work (Ref 2). Concerning
the problem of the tensions between the molecules, the author
refers to the work by V. A. Kargin and G. L. Slonimskiy (Ref 3).
With respect to the globular proteins, the determination of
the form and the dimensions was achieved for a great number
of objects. Furthermore, the author gives a relative character-
istic of the physical methods of the structural investigation
of high-molecular substances. The author considers the work-
ing out of a method for the detailed characteristic of the

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The Problem of the Structure of High-Molecular Substances

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degree of order of the molecules in polymeric compounds to be one of the most important problems in the field of the structure of high-polymeric substances. The author further found out that the investigations in the field of the structure of high-polymeric substances in the Soviet Union are not carried out with the necessary impetus. He regrets that nobody is occupied with the structural investigation of globular albuminous substances by means of diffraction methods which are of greatest importance for biology. The author is satisfied that the first steps in the field of the investigation of albuminous substances were carried out by means of the electron-resonance-method. He also finds backwardness in the field of albumin-radiography. According to his opinion, at least 2 research centers for albuminous structure ought to be established. In the field of the investigation of synthetic fiber and other high-polymeric substances it looks much better due to the systematic work carried out by V. A. Kargin and his collaborators, but also here he states the lack of a corresponding laboratory. The

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The Problem of the Structure of High-Molecular Substances   SOV/ 30-58-6-4/45

Laboratory of the Institute of High-Molecular Compounds, AS USSR in Leningrad, is under construction at present and cannot meet all requirements. The existing laboratories for the investigation of synthetic materials must be reinforced. There are 4 references, 3 of which are Soviet.

1. Synthetic materials--Structural analysis   2. Synthetic materials --Development   3. Molecular sturcture--Analysis

Card 4/4

AUTHORS: Kitaygorodskiy, A. I., Knyukh, Yu. V.   SOV/20-121-1-31/55

TITLE: A Triclinic Modification of Polythene (Triklinnaya
modifikatsiya politena)

ABSTRACT: 1) Molecules of the paraffin type may crystallize either in a
triclinic (T), monoclinic (M), or rhombic (R) form (Ref 1).
Triclinic subcells were found in normal paraffins with an
even atomic number of carbons from C_{18} to C_{26} and in some
normal sebacic acids, and others, whereas rhombic were found
in the case of polythene and other straight paraffins of C_{28}
and in the case of some normal sebacic acids. Substances with
monoclinic subcells have hitherto not been found. The differ-
ence in free energy between the packing R and T is not great.
Even several percents of admixtures of adjacent homologues
cause the transformation of the triclinic structure of an
n-paraffin to a rhombic one. The packing in the T-subcell has
the highest density of all possible packing types, the R-sub-
cell has, however, a higher symmetry. The probable existence

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A Triclinic Modification of Polythene   SOV/20-121-1-31/55

of the triclinic polythene modification was already earlier
pointed out on the strength of the analysis of the packing of
long chain molecules (Ref 4). 2) As far as the T-subcell has
a high coating density we may assume that this strength is
possible only in polythene samples with perfect structure, i.e.
the cleanest and with a minimum number of side ramifications.
A Debye-Scherer X-ray diagram gave an image which is character-
istic of a two phase system R + T. The modification occurred
in a smaller quantity than the rhombic one. Figure 1 shows the
last mentioned X-ray diagram and another one for the phase
diagram of n-paraffins (Ref 5). The measurement of interplanar
spacings and the comparison of the intensities confirmed final-
ly the existence of the triclinic modification of polythene
under normal conditions (Table 1). If the obtained results are
compared with the data from the investigation of the n-paraffin
C_{30} under high pressure (personal note of S. S. Kabalkina and

L. F. Vereshchagin) a second phase is detected beside the
rhombic one (Table 1) in $n-C_{30}$. Thus the existence of the tri-

clinic polythene modification which was assumed earlier by the
authors was proved. There are 1 figure, 1 table, and 6 refer-
ences, 4 of which are Soviet.

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A Triclinic Modification of Polythene   SOV/20-121-1-31/55

ASSOCIATION: Institut elemetoorganicheskikh soyedineniy Akademii nauk SSSR
                (Institute of Elementary Organic Compounds AS USSR)

PRESENTED: March 1, 1958, by V. A. Kargin, Member, Academy of Sciences,
                USSR

SUBMITTED: February 28, 1958

                1. Methanes—Crystallization   2. Methanes—Molecular structure
                3. Methanes—X-ray analysis

Card 3/3

AUTHORS: Kitaygorodskiy, A. I., Mnyukh, Yu. V. SOV/20-121-2-27/53

TITLE: The Variation of the Intermolecular Distances in Paraffin n-C$_{30}$H$_{62}$ With Temperature. Refining of the Molecule Form of the Paraffins (Temperaturnyye izmeneniya mezhmolekulyarnykh rasstoyaniy v parafine n-C$_{30}$H$_{62}$. Utochneniye formy molekuly parafinov)

PERIODICAL: Doklady Akademii nauk SSSR, 1958, Vol 121, Nr 2, pp. 291 - 294 (USSR)

ABSTRACT: In the present paper a report is given on investigations of the subcells of normal paraffins. 2 forms of such subcells are known: The orthorhombic cell (R) and the triclinic (T) one (Refs 1,2). The purpose of the investigations was to explain details of the structures and to determine the distances between the separate H-molecules. The investigation was limited to: n-C$_{30}$-paraffin (R-subcells), n-C$_{18}$-paraffin (T-subcells), normal fatty acids (basic pattern of the packing as in normal paraffin, but steric hindrance because of the COOH-group, therefore packing frequently diverging from paraffin), penta decanoic

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The Variation of the Intermolecular Distances in Paraffin $n\text{-}C_{30}H_{62}$ With Temperature. Refining of the Molecule Form of the Paraffins

acid (T-subcell, with $a=5,01$ Å and $b=4,25$ Å), and iodoform ($J_1 - J_1' = 3,98$ Å, $J_2 - J_2' = 4,34$ Å). For $n\text{-}C_{30}$-paraffin was obtained:

Distance between	$(+52^\circ)$	$(+20^\circ)$	extrapolated to -273°
$H_1 - H_3$	2,53	2,48	2,34
$H_1 - H_4$	2,95	2,92	2,86
$H_2 - H_4$	2,92	2,86	2,74
$H_2 - H_5$	2,43	2,42	2,36

There are 4 figures, 1 table, and 7 references, 4 of which are Soviet.

ASSOCIATION: Institut elementoorganicheskikh soyedineniy Akademii nauk SSSR (Institute of Elemental Organic Compounds, AS USSR)

Card 2/2

AUTHOS: Gonikberg, M. G., Kitaygorodskiy, A. I.   SOV/20-122-2-18/42

TITLE: On the Influence of Pressure Upon the Rate of Sterically
           Inhibited Reactions (K voprosu o vliyanii davleniya na
           skorost' prostranstvenno zatrudnennykh reaktsiy)

PERIODICAL: Doklady Akademii nauk SSSR, 1958, Vol 122, Nr 2,
           pp 231 - 234 (USSR)

ABSTRACT: The scarcely available experimental evidences suggest
           a considerable acceleration of the sterically inhibited
           reactions under increased pressure. Thus, tetramethyl
           ethylene was totally polymerized within 3 hours at 23,000
           atmospheric excess pressure, and at 300° whereas at 200°
           atmospheric excess pressure this was possible for 20% only.
           (Ref 1). The pressure also accelerates the thermal trans-
           formations of tetrachloro-ethylene at 300° and leads to
           the formation of hexachloro-butadiene and hexachloro-ethane
           (Ref 2). In both of these cases, the acceleration of
           reaction is but little related with the increasing con-
           centration of the initial material. It is, however, caused
Card 1/4   by an increased velocity constant of the reaction by the

On the Influence of Pressure Upon the Rate of   SOV/20-122-2-16/42
Sterically Inhibited Reactions

increase of pressure. In the present paper only the
values $\Delta v_{mol}^{\neq}$ are discussed (change in volume of the
reactive molecules at the formation of the activated
complex). Obviously, this value is an essential component
of the quantity

$\Delta v^{\neq}$ .The authors confine their discussion to the reactions
of Menshutkin which, by the way, were the object of various
kinetic investigations at high pressure. They proceed
from the conception of the structure of an activated
complex as it is seen from the scheme (Fig 1, Ref 5). Then,
reactions with pyridine, trimethylamine, and dimethyl-
aniline are discussed. The values computed according to
the scheme ($-\Delta v_{mol}^{\neq}$) reach some dozens cm^3 pro mol

for some Menshutkin reactions. With increasing pressure,
this must lead to a considerable acceleration of these
reactions according to the equation

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On the Influence of Pressure Upon the Rate of
Sterically Inhibited Reactions   SOV/20-122-2-18/42

$$\left(\frac{d \ln K}{dp} \right)_T = - \frac{\Delta v^{\neq}}{RT}$$ (1). By the results of table 1
it becomes evident that the acceleration really occurs.
The qualitative determination of a sterically inhibited
formation process of an activated complex makes it possible
to explain the various accelerations of the Menshutkin
reactions by pressure if these reactions differ by the
structure of the participating amines and haloid alkyls.
In particular, the increasing acceleration of these reactions
with the transition of CH_3J to C_2H_5J and to iso-C_3H_7J as
well as of C_5H_5N to $(CH_3)_3N$ and to $C_6H_5N(CH_3)_2$ becomes
clear, further the same pressure effect in the reactions
of trimethylamine and triethylamine. Of course, for a
perfect analysis of the influence of pressure upon the
velocity of the reaction, all $\Delta v^{\neq}$ are to be considered.
There are 3 figures, 1 table, and 11 references, 3 of which
are Soviet.

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On the Influence of Pressure Upon the Rate of   S0V/2o-122-2-18/42
Sterically Inhibited Reactions

ASSOCIATION: Institut organicheskoy khimii im.N.D.Zelinskogo Akademii nauk
              SSSR (Institute of Organic Chemistry imeni N.D.Zelinskiy, AS USSR)

              Institut elementoorganicheskikh soyedineniy Akademii nauk SSSR
              (Institute of **Elementary Organic Compounds, AS USSR**)

PRESENTED: April 29, 1958, by B.A.Kazanskiy, Member, Academy of Sciences,
             USSR

SUBMITTED: April 24, 1958

Card 4/4

KITAYGORODSKIY, A. I.; STRUCHKOV, Yu. T.; KHOTSYANOVA, Tat'yana L'vovna:
VOL'PIN, M. Ye.; KURSANOV, D. N.

"The Crystal Structures of Tropylium Perchlorate and Iodide"

a report presented at Symposium of the International Union of
Crystallography   Leningrad, 21-27 May 1959

KITAYGORODSKIY, ALEKSANDR ISAAKOVICH

"Strains and Conformations of Organic Molecules "

A paper/report presented at Symposium of the International Union of
Crystallography, Lenningrad   21-27 May 1959

SO: B, 3,135,471   28 July 1959

PHASE I BOOK EXPLOITATION   SOV/3930

Kitaygorodskiy, Aleksandr Isaakovich

Poryadok i besporyadok v mire atomov (Order and Disorder in the World of Atoms) 3rd ed., enl. Moscow, Fizmatgiz, 1959. 150 p. 18,000 copies printed.

Ed.: A.L. Leshchinskiy; Tech. Ed.: A.P. Kolesnikova.

PURPOSE: This book is intended for the general reader with an elementary knowledge of physics.

COVERAGE: The book discusses the three states of matter, solid, liquid and gas, and its transformation by liquefaction, evaporation, etc. These processes are examined from the point of view of order or disorder in atoms. Such an interpretation of atomic structure is thought appropriate as some substances are arrangements of particles that can be described as either "orderly" or "disorderly;" others are characterized as both "orderly and disorderly" and in these the two are inseparable. Transformations in metals, plastics, or rubber in such technological processes as hardening or mechanical working also produce changes in the order of the distribution of atoms. Thus, the problem of order and disorder in

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Order and Disorder in the World of Atoms   SOV/3930

atoms is a large part of the study of the structure and properties of substances.
The book is written in a popular style and contains 65 diagrams and sketches.
No personalities are mentioned. There are no references.

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